Supplementary Information

The composition dependence of Glass forming propensity in Al-Ni alloys

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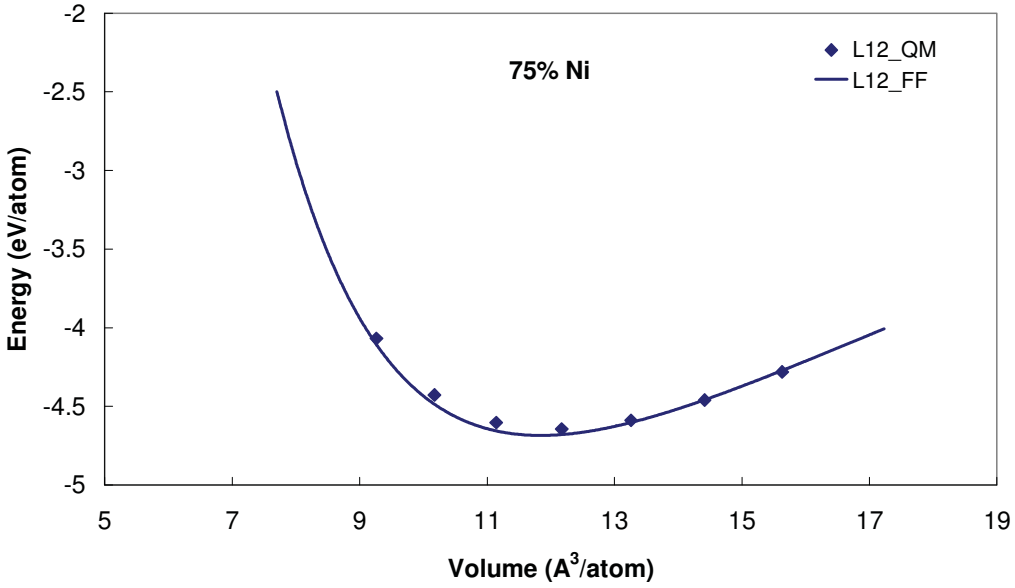
FIG. S1 Equation of states at 5 compositions (a) 75% Ni, (b) 62.5%Ni, (c) 50%Ni, (d) 40% Ni, (e) 25% Ni. (Dots are QM data, and lines are results from the GRL Force Field.)

FIG. S2. Density of States from 2PT analysis for different phases of AlNi (a) B2 structure at 100K; (b) B2 structure at 1000K; (c) liquid at 2200K; (d) amorphous phase at 100K.

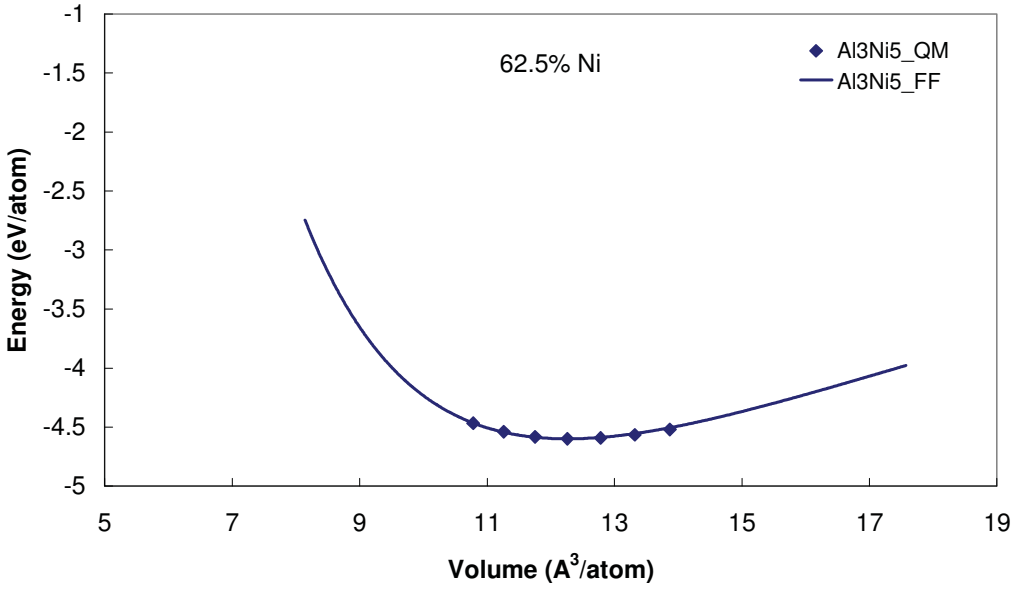
FiG.S3. Variation of the fractions of Honeycutt-Andersen indices of $AlNi_3$ during (a) heating and (b) cooling at $4x10^{12}$ K/s.

FIG. S4. Density of States from 2PT analysis for different phases of $AlNi_3$ at 100K. (a) $L1_2$ structure; (b) partially disordered fcc structure obtained from cooling the melt at rate of $4x10^{12}$ K/s.

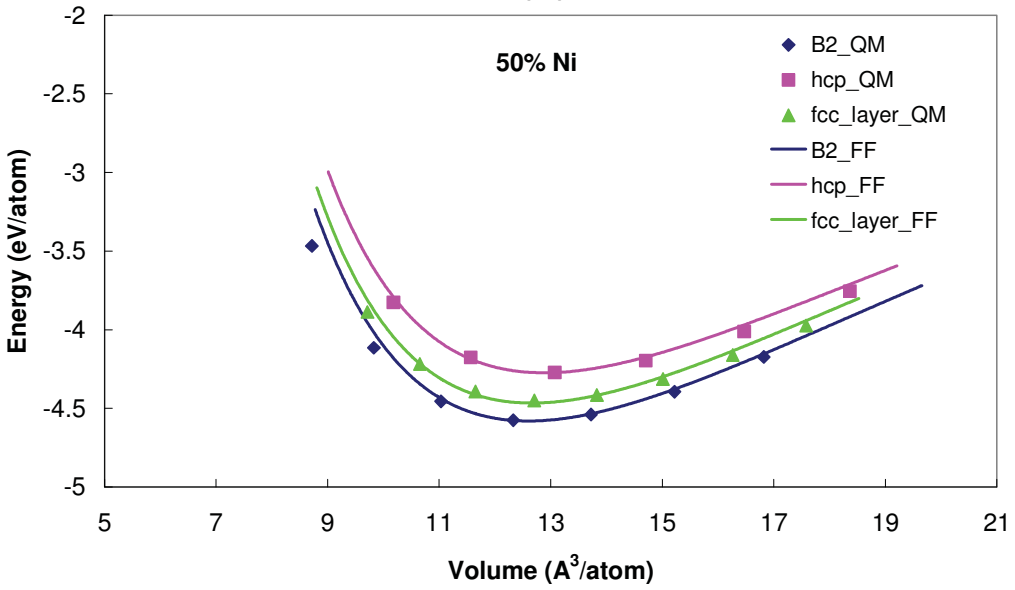
(a)


75% Ni
L12_QM
L12_FF
Energy (eV/atom)
-2
-2.5
-3
-3.5
-4
-4.5
-5
5
7
9
11
13
15
17
19
Volume (A3/atom)

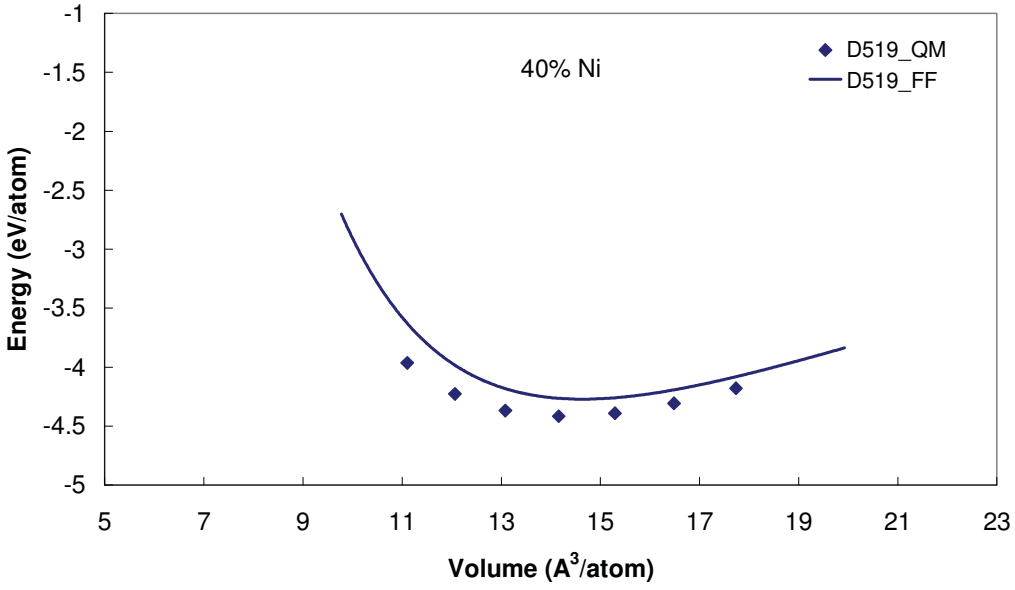
(b)

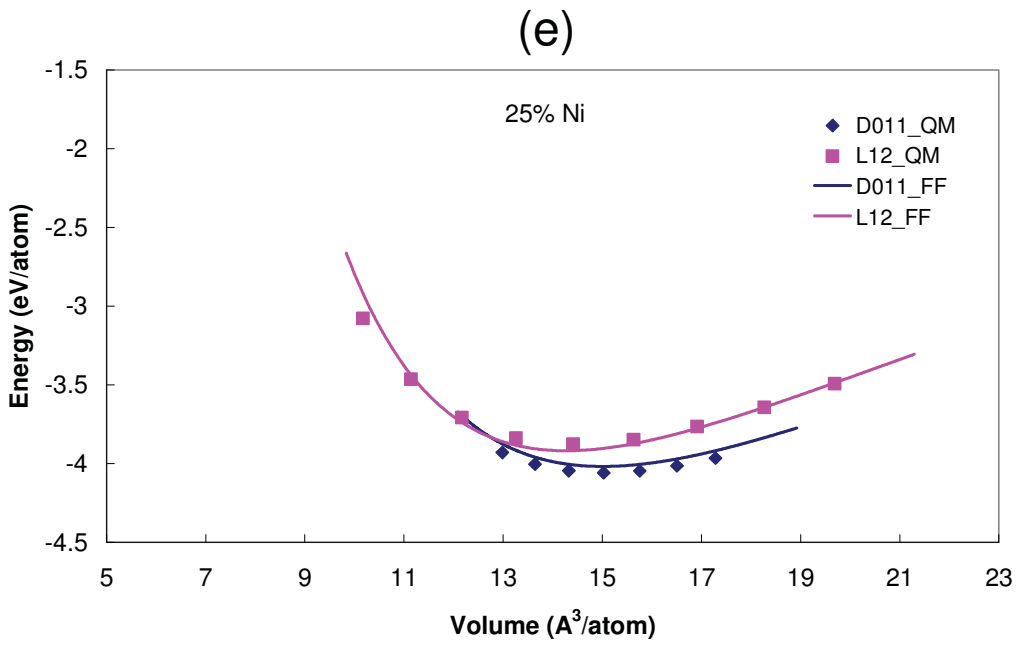

62.5% Ni
Al3Ni5_QM
Al3Ni5_FF
Energy (eV/atom)
-1
-1.5
-2
-2.5
-3
-3.5
-4
-4.5
-5
5
7
9
11
13
15
17
19
Volume (A3/atom)

(c)


50% Ni
B2_QM
hcp_QM
fcc_layer_QM
B2_FF
hcp_FF
fcc_layer_FF
Energy (eV/atom)
-2
-2.5
-3
-3.5
-4
-4.5
-5
5
7
9
11
13
15
17
19
21
Volume (A3/atom)

(d)


40% Ni
D519_QM
D519_FF
Energy (eV/atom)
-1
-1.5
-2
-2.5
-3
-3.5
-4
-4.5
-5
5
7
9
11
13
15
17
19
21
23
Volume (A3/atom)



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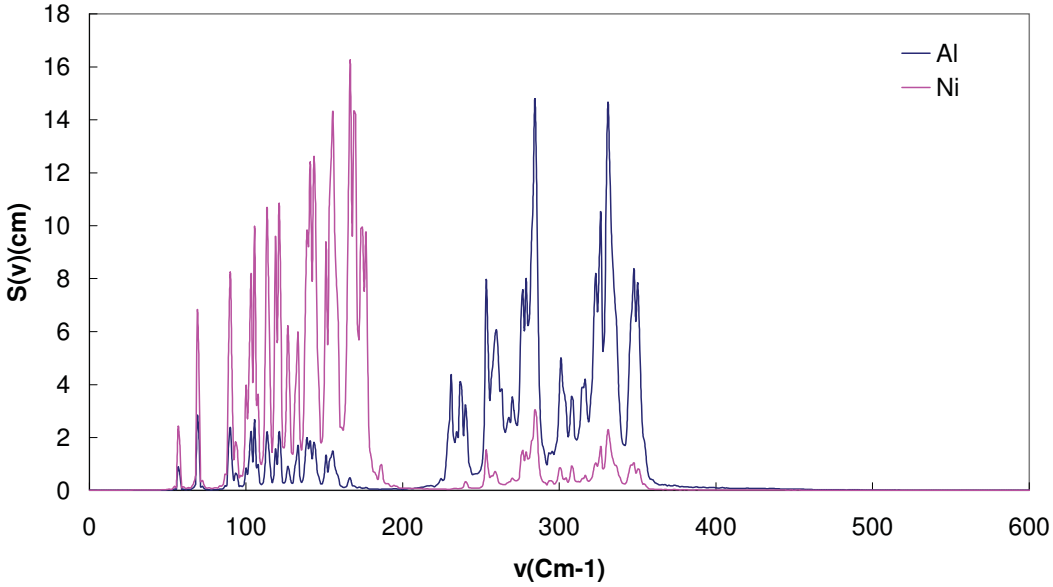
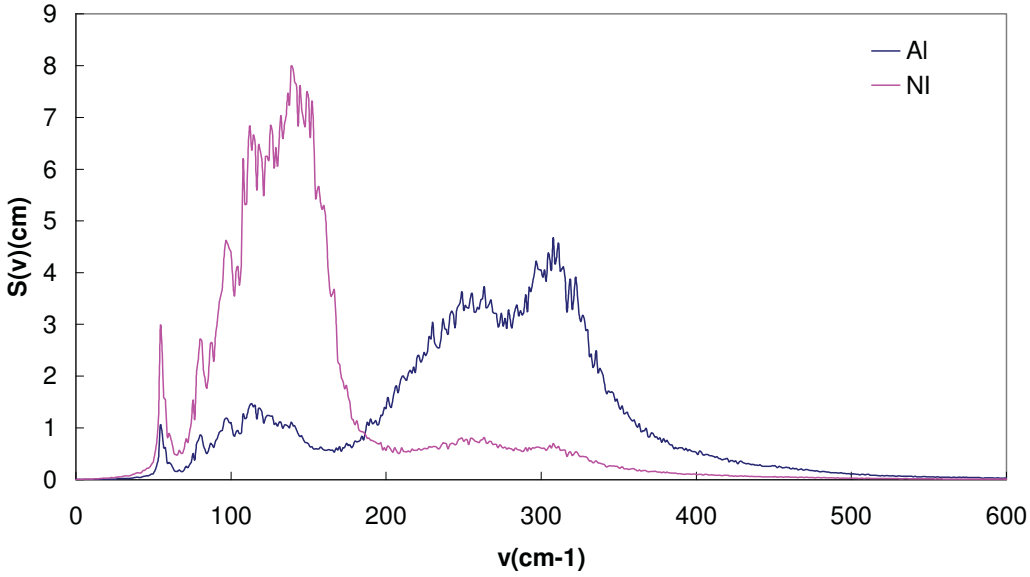
(a)


Al
Ni
S(v)(cm)
v(Cm-1)
0
2
4
6
8
10
12
14
16
18
0
100
200
300
400
500
600

(b)


Al
NI
S(v)(cm)
v(cm-1)
0
1
2
3
4
5
6
7
8
9
0
100
200
300
400
500
600

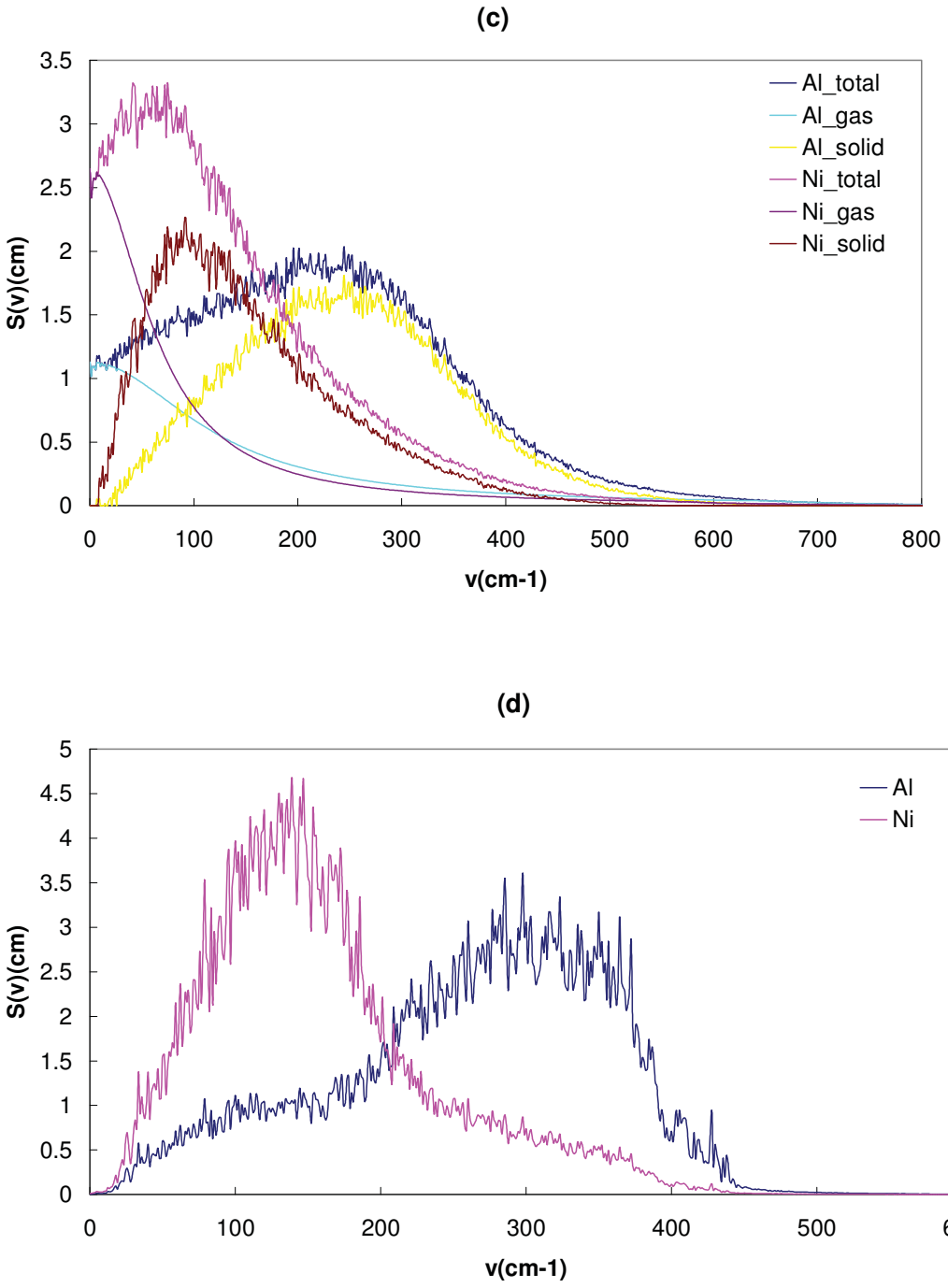


FIG. S2. Density of States from 2PT analysis for different phases of AlNi. (a) B2 structure at 100K; (b) B2 structure at 1000K; (c) liquid at 2200K; (d) amorphous phase at 100K.

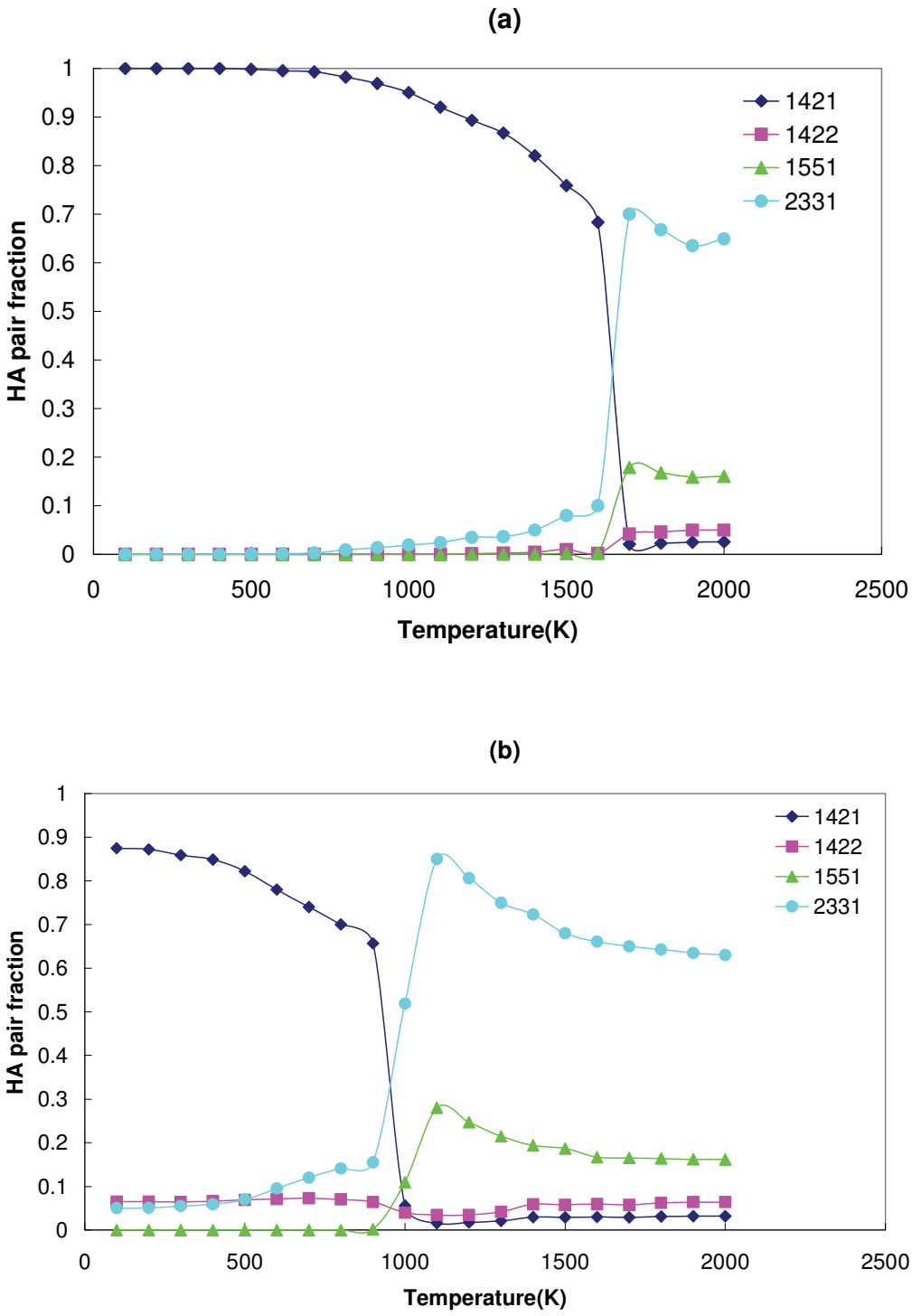
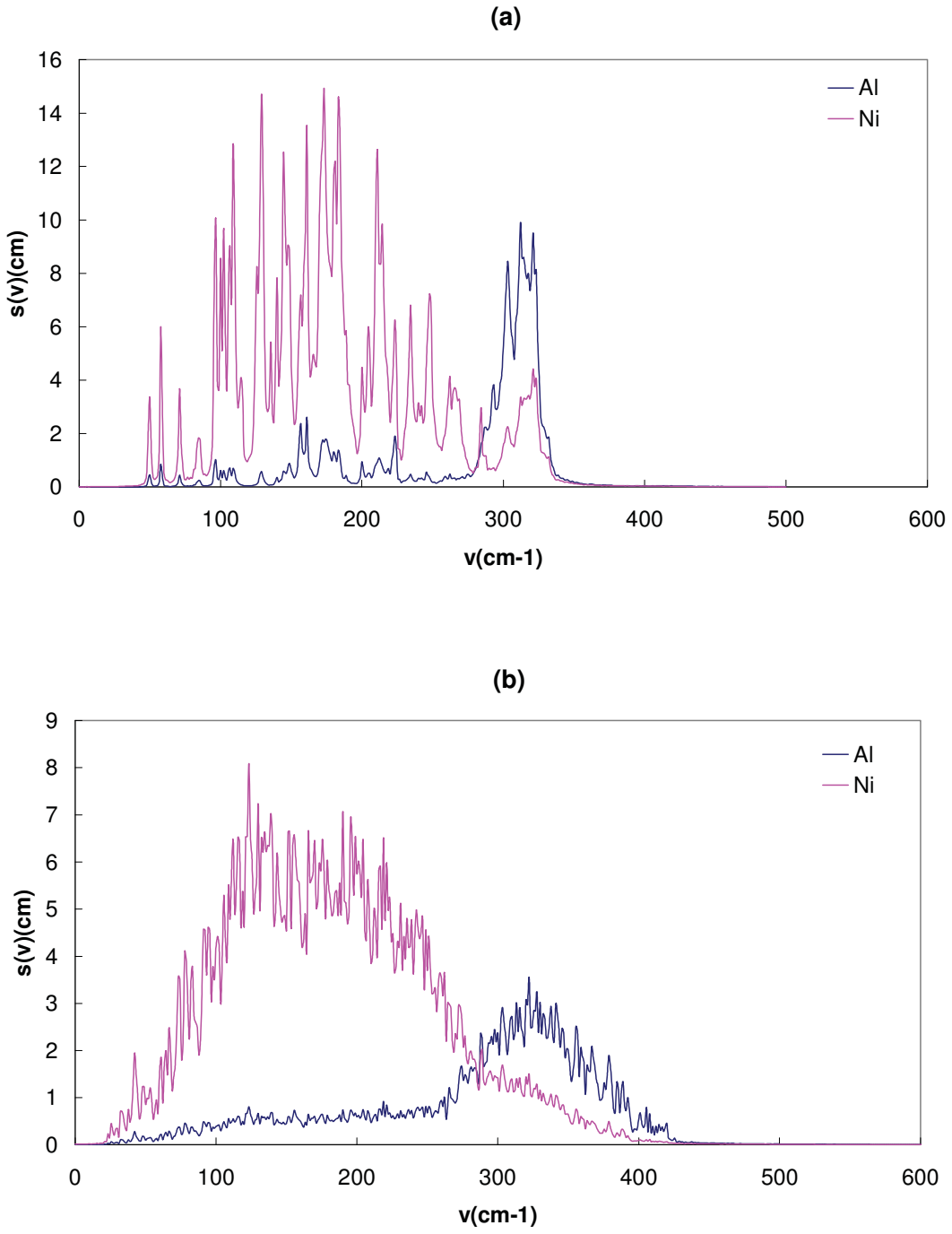


Fig. S3. Variation of the fractions of Honeycutt-Andersen indices of $AlNi_3$ during (a) heating and (b) cooling at $4x10^{12}$ K/s.



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